CURRICULUM VITAE OF QUANLIN ZHOU

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1. EDUCATION AND DEGREES

1996 – 1999	Ph.D. in Civil & Environmental Engineering Technion-Israel Institute of Technology, Haifa, Israel
1987 – 1990	M. Eng. in Hydrology and Water Resources Hohai University, Nanjing, China.
1983 – 1987	B. Eng. in Hydrology and Water Resources Hohai University, Nanjing, China

2. EMPLOYMENT HISTORY

11/2008 – Present	Geological Research Scientist (Career)
06/2006 – 10/2008 09/2002 – 06/2005	Geological Research Scientist (Career-Track)
03/2001 – 09/2002	Geological Postdoctoral Fellow
	Earth Sciences Division Lawrence Berkeley National Laboratory (LBNL) University of California 1 Cyclotron Road, MS90-1116, Berkeley, CA 94720
06/2005 – 06/2006	Senior Modeler, ETIC Engineering Inc. 1333 Broadway, Suite 1015, Oakland, CA 94612
10/2000 – 03/2001	Postdoctoral Fellow, Department of Geology & Geophysics University of Wisconsin at Madison 1215 W. Dayton Street, Madison, WI53706
10/1999 – 09/2000	Postdoctoral Associate Department of Civil & Environmental Engineering, MIT 15 Vassar Street, Cambridge, MA 02139
10/1995 – 10/1996	Senior Engineer
07/1990 – 10/1995	Engineer
	Nanjing Institute of Hydrology and Water Resources Ministry of Water Resources, Nanjing, China

3. RESEARCH EXPERIENCE

3.1 Research Interests:

- Analytical and numerical modeling of flow and contaminant transport in fractured/porous media for nuclear waste disposal, geologic carbon sequestration, and site-specific contamination remediation
- Multiphase and unsaturated flow in heterogeneous fractured/porous media; preferential flow, lateral spreading, upscaling and effective properties
- Geologic carbon sequestration: pressure buildup and brine migration and their impact on groundwater resources at basin scale; enhanced storage capacity and safety in natural hierarchical, multiscale, heterogeneous sedimentary rocks at plume scale; early leakage detection by joint inversion of reservoir/overburden pressure and land surface uplift
- Diffusive transport in fractured rock and layered porous media at small and field scales; behavior of field-scale effective diffusion coefficient for heterogeneous media; effective diffusion in unsaturated and multiphase flow conditions
- Characterization of large-scale contaminant plumes, with physical, chemical, microbial (biodegradation) processes; conceptual understanding with detailed data and inverse analysis in support of on-site remediation and natural attenuation
- Density-dependent flow for seawater intrusion and brine transport
- Software development of FEAS, a highly integrated C++ code family, for simulation of various kinds of coupled (and uncoupled) flow and transport.

3.2 Research Proposals Funded (Total Funds: $10.6M, Total Funds as PI and Co-PI: $10.1M):

Projects for Geologic Carbon Sequestration (FY2008 – FY2018) (Total Funding: $10.35M)

1. Large-scale hydrologic impacts of CO_2 geological storage (FY2010 – FY2012, Co-PI with Jens Birkholzer, **$1,141K** funded by USDOE) ($375K in FY10 + $386K in FY11 + $380K in FY12)
2. Joint inversion of monitoring data for early leakage detection (FY2011 – FY2015, Co-PI with Michael Kowalsky, **$2,000K** funded by USDOE)
3. Modeling and monitoring support of the Big Sky Partnership's Phase III project at Kevin Dome (FY2011 – FY2018, Co-PI with Curtis Oldenburg, and Task Lead for modeling, **$5,560K** funded by USDOE)
4. Collaboration with China on geologic carbon sequestration: Novel field tests to characterize heterogeneity for China's first pilot test (FY2011 – FY2012, PI, **$350K**, LDRD, funded by Lawrence Berkeley National Laboratory)
5. Analytical and numerical modeling in support of EPA Area-of-Review estimates and geologic sequestration modeling framework (2008-2012, PI, a total of **$447.5K** funded by USEPA) ($75K in 2008 + $160K in 2010 + $212.5K in 2011)
6. Potential impacts of future geological storage of CO_2 on the groundwater resources in California's Central Valley (September 2010 – May 2013, Co-PI with Preston Jordan, **$490K** funded by California Energy Commission, CEC)

7. Validation of models simulating capillary and dissolution trapping during injection and post-injection of CO_2 in heterogeneous geological formations using data from intermediate scale test systems (FY2011 – FY2013, $600K funded by USDOE, LBNL share of **$150K**)
8. Modeling support of the FutureGen Carbon Sequestration project (FY2011 – FY2012, **$210K** funded by the FutureGen Alliance)

Other Projects (2007-2009) (Total Funding: $242K)

9. Coupling state-of-the-science subsurface simulation with advanced user interface and parallel visualization (2007, PI, $100K funded by DOE Office of Science, LBNL share: **$32K**)
10. Photo- and bio-degradation of N-nitrosodimethylamine (NDMA) in a coupled surface water and groundwater system in Montebello Forebay, California (2007, PI, **$50K** funded by Los Angeles County of Sanitation Districts)
11. Mobility of tritium in engineered and earth materials at the NuMI facility, Fermilab, Phase II (2007-2009, **$160K** funded by Fermi National Accelerator Laboratory, PI: Stefan Finsterle)

3.3 Previous Research Projects:

- Large-scale hydrological evaluation and modeling of the impact of CO_2 geological sequestration on groundwater systems (Completed at LBNL, FY2006-FY2009)
- Calibration of unsaturated zone properties for the Yucca Mountain Project, with the resultant ANL-NBS-HS-000058 Rev 00 report (completed at LBNL, 2007)
- Dissolved TCE transport in a weathered, fractured rock zone at Charlotte, North Carolina: evidence of back diffusion from matrix to fractures from remediation of a long-term TCE plume (completed at ETIC, 2006)
- Scale-dependence of field-scale, effective matrix diffusion coefficient in fractured media: enhanced retardation of solute/radionuclide transport (completed at LBNL, 2005)
- Investigation of flow focusing in heterogeneous fractured rock at Yucca Mountain, Nevada (completed at LBNL, 2004)
- Analysis of fracture-informed spatial variability of infiltration and seepage in fractured rock at Yucca Mountain, Nevada (completed at LBNL, 2004)
- Pretest prediction for the Alcove 8–Niche 3 field seepage and tracer tests conducted in two tunnels at Yucca Mountain, Nevada (completed at LBNL, 2003)
- Modeling groundwater flow and advective transport at the contaminated LBNL site in support of on-site remediation (completed at LBNL, 2003)
- International co-operative project for the development of coupled thermo-hydro-mechanical (THM) models and their validation against experiments in nuclear waste isolation (DECOVALEX) (completed at LBNL, 2002)
- Effects of multiscale heterogeneity of hydrogeologic properties on unsaturated flow and transport in fractured rock at Yucca Mountain, Nevada (completed at LBNL, 2001)
- Effective properties of multiphase flow in heterogeneous porous media (completed at MIT, 2000)
- Modeling of seawater intrusion in coastal aquifers (completed at Technion,1996-1999)

- Modeling of strongly coupled density-dependent flow and salt transport (completed at Technion, 1996-1999)
- Development and application of FEAS, a highly integrated C++ code family, for various complex, coupled, nonlinear transport phenomena in subsurface systems (1996-2008)
- Real-time control of main canal and optimal operation of water supply and distribution in the Middle Route of the South-To-North Water Transfer Project (SNWTP-MR) (completed in China, 1995-1996)
- Risk analysis of flood control benefits of the Three-Gorge Project (completed in China, 1991)

4. AWARDS AND PROFESSIONAL SOCIETIES

- "Outstanding Performance Award," Lawrence Berkeley National Laboratory, 2007
- "The Miriam and Aaron Gutwirth Award," the Gutwirth Foundation, Israel, 1999
- "The Irmay Prize," Department of Civil Engineering, Technion-Israel Institute of Technology, Haifa, Israel, 1998
- Reviewers for top journals in hydrogeology (44 times), one book chapter, and one book (updated on 07/01/2011):
    - Water Resources Research (9 times),
    - Advances in Water Resources (1)
    - Transport in Porous Media (17),
    - Journal of Contaminant Hydrology (2),
    - Ground Water (5),
    - Journal of Hydrology (2),
    - Hydrogeology Journal (3),
    - Environmental Science & Technology (1),
    - International Journal of Greenhouse Gas Control (2)
    - Journal of Geotechnical and Geoenvironmental Engineering (1),
    - Computers and Geosciences (1)
    - AGU Monograph book chapter (1).
    - Book: "Geological storage of CO2: Modeling Approaches for Large-Scale Simulation" by Jan M. Nordbotten and Michael A. Celia.
- Member, American Geophysical Union, Geological Society of America
- Supervisor of two postdoctoral fellows

5. REFERENCES

Prof. Jacob Bear

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6. SCIENTIFIC AND PROFESSIONAL PUBLICATIONS

6.1 Peer-Reviewed Journal Publications [Total SCI Citations: 177, H-Index = 9]

J1. Cihan, A., **Q. Zhou**, and J. T. Birkholzer, 2011. Analytical solutions for pressure perturbation and fluid leakage through aquitards and wells in a multilayered system, *Water Resources Research* (in press)

J2. Birkholzer, J.T., J.-P. Nicot, C. M. Oldenburg, **Q. Zhou**, S. Kraemer, K. Bandilla, 2011. Brine flow up a well caused by pressure perturbation from geologic carbon sequestration: Static and dynamic evaluations, *International Journal of Greenhouse Gas Control* 5, doi:10.1016/j.ijggc.2011.01.003. [LBNL-4864E]

J3. **Zhou, Q.**, and J. T. Birkholzer, 2011. On scale and magnitude of pressure build-up induced by large-scale geologic storage of CO_2, *Greenhouse Gases: Science and Technology* 1, 11-20, DOI: 10.1002/ghg3.001. [LBNL-4898E]

J4. **Zhou, Q.**, J. T. Birkholzer, and C.-F. Tsang, 2011. Reply to Comments by Veling on "A Semi-Analytical Solution for Large-Scale Injection-Induced Pressure Perturbation and Leakage in a Laterally Bounded Aquifer-Aquitard System" by Zhou, Birkholzer, and Tsang, *Transport in Porous Media* 86, 357-358. [LBNL-4896E]

J5. **Zhou, Q.**, J. T. Birkholzer, E. Mehnert,Y.-F. Lin, and K. Zhang, 2010. Modeling basin- and plume-scale processes of CO_2 storage for full-scale deployment, *Ground Water*, 48(4), 494-514. [LBNL-2788E, SCI Citations: 3]

J6. Birkholzer, J.T., and **Q. Zhou**, 2009. Basin-scale hydrogeologic impacts of CO_2 storage: Regulatory and capacity implications, *International Journal of Greenhouse Gas Control* 3 (6), 745–756 [LBNL-1716E, SCI Citations: 11].

J7. **Zhou, Q.**, S. McCraven, J. Garcia, M. Gasca, T. A. Johnson, and W. Motzer, 2009. Field evidence of biodegradation of N-Nitrosodimethylamine (NDMA) in groundwater with incidental and active recycled water recharge, *Water Research* 43(3), 793-805 [SCI Citations: 4].

J8. **Zhou, Q.**, J. T. Birkholzer, and C.-F. Tsang, 2009. A semi-analytical solution for large-scale injection-induced pressure perturbation and leakage in a laterally bounded aquifer-aquitard system, *Transport in Porous Media*, 78(1), 127-148. [LBNL-1021E, SCI Citations: 3]

J9. Birkholzer, J.T., **Q. Zhou**, and C.-F. Tsang, 2009. Large-scale impact of CO_2 storage in deep saline aquifers: A sensitivity study on pressure response in stratified systems, *International Journal of Greenhouse Gas Control* 3, 181-194. [LBNL-1252E, SCI Citations: 23]

J10. **Zhou, Q.**, J. T. Birkholzer, C.-F. Tsang, and J. Rutqvist, 2008. A method for quick assessment of CO_2 storage capacity in closed and semi-closed saline aquifers, *International Journal of Greenhouse Gas Control* 2, 626-639. [LBNL-63820, SCI Citations: 26]

J11. Guan, J., F. J. Molz, **Q. Zhou,** H.-H. Liu, and C. Zheng, 2008. Behavior of the mass transfer coefficient during the MADE-2 experiment: New insights, *Water Resources Research* 44, W02423, doi:10.1029/2007WR006120. [LBNL-63023, SCI Citations: 6]

J12. Su, G.W., J. Jasperse, D. Seymour, J. Constantz, and **Q. Zhou**, 2007. Simulation analysis of pumping-induced unsaturated regions beneath a perennial river, *Water Resources Research* 43, W08421, doi:10.1029/2006WR005389. [LBNL-63048, SCI Citations: 5]

J13. **Zhou, Q.**, H.-H. Liu, F. J. Molz, Y. Zhang, and G. S. Bodvarsson, 2007. Field-scale effective matrix diffusion coefficient for fractured rock: Results from literature survey, *Journal of Contaminant Hydrology* 93, 161–187. [LBNL-57368, SCI Citations: 14]

J14. Liu, H.-H., Y. Zhang, **Q. Zhou,** and F. J. Molz, 2007. An interpretation of potential scale dependence of the effective matrix diffusion coefficient, *Journal of Contaminant Hydrology* 90, 41-57. [LBNL-60744, SCI Citations: 12]

J15. Zhang, Y., H.-H. Liu, **Q. Zhou**, and S. Finsterle, 2006. Effects of diffusive property heterogeneity on effective matrix diffusion coefficient for fractured rock, *Water Resources Research* 42, W04405, doi:10.1029/2005WR004513. [LBNL-58695, SCI Citations: 5]

J16. **Zhou, Q.**, H.-H. Liu, G. S. Bodvarsson, and F. J. Molz, 2006a. Evidence of multi-process matrix diffusion in a single fracture from a field tracer test, *Transport in Porous Media* 63(3), 473–487. [LBNL-58198, SCI Citations: 10]

J17. **Zhou, Q.**, R. Salve, H.-H. Liu, J. Wang, and D. Hudson, 2006b. Analysis of a meso-scale infiltration and water seepage test in unsaturated fractured rock: Spatial variabilities and discrete fracture patterns, *Journal of Contaminant Hydrology* 87, 96-122. [LBNL-55489, SCI Citations: 4]

J18. **Zhou, Q.**, J. Bear, and J. Bensabat, 2005. Saltwater upconing and decay beneath a well pumping above an interface zone, *Transport in Porous Media* 61(3), 337-363. [LBNL-55486, SCI Citations: 10]

J19. **Zhou, Q.**, J. T. Birkholzer, I. Javandel, and P. D. Jordan, 2004. Modeling three-dimensional groundwater flow and advective contaminant transport at a heterogeneous mountainous site in support of remediation, *Vadose Zone Journal* 3, 884–900. [LBNL-54318, SCI Citations: 2]

J20. **Zhou, Q.**, H.-H. Liu, G. S. Bodvarsson, and C. M. Oldenburg, 2003. Flow and transport in unsaturated fractured rocks: Effects of multiscale heterogeneity of hydrogeologic properties, *Journal of Contaminant Hydrology* 60 (1-2), 1-30. [SCI Citations: 20]

J21. **Zhou, Q.**, J. Bensabat, and J. Bear, 2001. Accurate calculation of specific discharge in heterogeneous porous media, *Water Resources Research* 37(12), 3057-3069. [SCI Citations: 2].

J22. Bensabat, J., **Q. Zhou**, and J. Bear, 2000. An adaptive pathline-based particle tracking algorithm for the Eulerian-Lagrangian method, *Advances in Water Resources* 23(4), 383-397. [SCI Citations: 16]

J23. Zhu, Y., and **Zhou, Q**., 1995. Risk analysis of flood control benefits of the Three-Gorge Project, *J. of Advances in Water Sciences (in Chinese)* 6(1), 29-35.

6.2 Book Chapters

B1. Karsten Pruess, Jens T. Birkholzer, and **Quanlin Zhou**, 2011. Mathematical models as tools for probing long-term safety of CO_2 storage, in *Developments and Innovation in Carbon Capture and Storage* (CCS) Technology (Maroto-Valer, M.M., ed.), Woodhead Publishing, Cambridge, UK (in press).

B2. Jacob Bear and **Quanlin Zhou**, 2007. Sea water intrusion into coastal aquifers, Chapter 12 in *the Handbook of Groundwater Engineering, Second Edition*, Jacques Delleur (editor), CRC Press, Taylor & Francis Group, Boca Raton, Florida. (LBNL-63047)

B3. Hui-Hai Liu, Jonny Rutqvist, **Quanlin Zhou,** and Gudmundur S. Bodvarsson, 2004. Upscaling of normal stress-permeability relationships for fracture networks obeying fractional Levy motion, in *Elsevier Geo-Engineering Book Series Volume II, Coupled Thermo-Hydro-Mechanical-Chemical Processes in Geo-Systems: Fundamentals, Modeling, Experiments and Applications*, by Stephansson, O., Hudson, J. A., Jing, L. (editors), Oxford, p. 263–268.

6.3 Conference Papers

C1. Illangasekare, T.H., Trevisan, L., Rodriguez, D., Sakaki, T., Cihan, A., Birkholzer, J.T., and **Zhou, Q.**, 2011. A fundamental study of migration and entrapment of supercritical CO_2 in heterogeneous deep geologic formations: Intermediate-scale testing and modeling, *the EGU 2011 Meeting*, Vienna, Austria, April 10-14, 2011.

C2. Trevisan, L.,Illangasekare, T.H., Rodriguez, D., Sakaki, T., Cihan, A., Birkholzer, J.T., and **Zhou, Q.**, 2011. Improved understanding of migration and entrapment of supercritical CO_2 in deep geologic formations: Intermediate-scale testing and modeling, *The MODFLOW and More 2011: Integrated Hydrologic Modeling*, Golden, CO, June 5-8, 2011.

C3. Murakami, H., S. Finsterle, **Q. Zhou**, J.T. Birkholzer, 2011. Uncertainty quantification and global sensitivity analysis of CO2 migration and pressure buildup for a hypothetical GCS project in the Southern San Joaquin Basin in California, *The Tenth Annual Carbon Capture & Sequestration*, May 2-5, Pittsburgh, PA.

C4. Cihan, A., **Q. Zhou**, J.T. Birkholzer, Analytical solutions for leakage through aquitards and abandoned wells in multilayered aquifer-aquitard systems, *The Tenth Annual Carbon Capture & Sequestration*, May 2-5, Pittsburgh, PA.

C5. Jens T. Birkholzer, JP Nicot, Curtis M. Oldenburg, Quanlin Zhou, Stephen Kraemer, Karl Bandilla, 2011. Brine leakage up a well caused by pressure perturbation from CO2 injection: A discussion of threshold pressures, flow rates, and environmental impact, *The Tenth Annual Carbon Capture & Sequestration,* May 2-5, 2011, Pittsburgh, PA.

C6. Birkholzer, J.T., **Q. Zhou,** L. Zheng, and N. Spycher, 2011. CO_2 geological storage and groundwater resources: Model applications, *the 2011 SIAM Conference on Mathematical and Computational Issues in Geosciences*, Long Beach, CA, March 21-24, 2011.

C7. Birkholzer, J.T., **Q. Zhou**, A. Cortis, and S. Finsterle, 2010 (Talk). A sensitivity study on regional pressure buildup from large-scale CO_2 storage projects, *the 10th International Conference on Greenhouse Gas Control Technologies (GHGT-10)*, Sept 19-23, 2010, Amsterdam, the Netherland.

C8. **Quanlin Zhou**, Jens T. Birkholzer, and Jeffrey L. Wagoner, 2010 (Talk). Modeling the potential impact of geologic carbon sequestration in the southern San Joaquin basin, California, *The Ninth Annual Carbon Capture & Sequestration*, May 10-13, Pittsburgh, PA

C9. **Quanlin Zhou** and Jens T. Birkholzer, 2010. The secondary seal effect on CO_2 plume development and migration in a sedimentary basin, *Caprocks and Seals for Geologic Carbon Sequestration*, January 12 to 15, 2010, Pacific Grove, CA.

C10. Jens T. Birkholzer and **Quanlin Zhou**, 2010. Large-scale impact of CO_2 storage in deep saline aquifers: The importance of caprock permeability, *Caprocks and Seals for Geologic Carbon Sequestration*, January 12 to 15, 2010, Pacific Grove, CA.

C11. Jens T. Birkholzer and **Quanlin Zhou**, 2009. An Integrated Model for Basin- and Plume-scale Processes Related to Full-Scale Employment of CO_2 Storage – The Illinois Basin as an Example, Extended Abstract, *AAPG/SEG/SPE Hedberg Conference on Geological Carbon Sequestration: Prediction and Verification*, Vancoucer, BC, Canada, August 16-19, 2009.

C12. **Quanlin Zhou,** Jens T. Birkholzer, Hannes Leetaru, Edward Mehnert, Yu-Feng Lin, 2009 (Talk). Integrated modeling of basin-scale impacts on groundwater resources and plume-scale transport behavior of geologic carbon sequestration in the Illinois sedimentary basin, *the 7th International Conference on Calibration and Reliability in Groundwater Modeling, Managing Groundwater and the Environment*, September 20-23, 2009, Wuhan, China.

C13. **Quanlin Zhou**, Jens T. Birkholzer, Edward Mehnert, and Yu-Feng Lin, 2009 (Talk). Basin-scale hydrological impact of geologic carbon sequestration in the Illinois Basin: A full-scale deployment scenario, *Water/Energy Sustainability Symposium at the 2009 Groundwater Protection Council Annual Forum*, September 13 to 16, Salt Lake City, Utah.

C14. **Quanlin Zhou**, Lehua Pan, James Hylen, Byron G. Lundberg, Robert K. Plunkett, Stephen H. Pordes, and Stefan A. Finsterle, 2009. Modeling of multiphase diffusive processes of tritium in an underground accelerator facility, *TOUGH Symposium 2009*, Berkeley, CA, September 14-16, 2009.

C15. Jens T. Birkholzer, and **Quanlin Zhou**, 2009. Integrated modeling of basin- and plume-scale processes related to geologic carbon sequestration in the Illinois Basin, *TOUGH Symposium 2009*, Berkeley, CA, September 14-16, 2009.

C16. **Quanlin Zhou**, Jens T. Birkholzer, Hannes Leetaru, Edward Mehnert, Yu-Feng Lin, 2009 (Invited Talk). Basin-scale environmental impact of geologic carbon sequestration: evaluation of a hypothetical scenario for full-scale deployment in the Illinois Basin, *The American Water Works Association (AWWA) Annual Meeting* in San Diego, CA, June 14-18, 2009.

C17. Jens T. Birkholzer and **Quanlin Zhou**, 2009 (Talk). Basin-scale hydrological impacts of multiple-site CO_2 storage in the Illinois Basin: Regulatory and capacity implications, *The Eighth Annual Conference on Carbon Capture & Sequestration*, Pittsburgh, PA, May 4-7, 2009.

C18. **Quanlin Zhou**, Jens T. Birkholzer, Hannes Leetaru, Edward Mehnert, Yu-Feng Lin, Chin-Fu Tsang, Preston Jordan, Scott Frailey, and Robert Finley, 2009 (Talk). Integrated modeling of basin-scale and plume-scale processes related to geologic carbon sequestration in the Illinois Basin, *The Eighth Annual Conference on Carbon Capture & Sequestration*, Pittsburgh, PA, May 4-7, 2009.

C19. **Quanlin Zhou**, Jens T. Birkholzer, Hannes Leetaru, Edward Mehnert, Chin-Fu Tsang, Scott Frailey, and Robert Finley, 2009 (Invited Talk). Basin-scale environmental impact of geologic carbon sequestration in the Illinois Basin*, the Symposium of Carbon Sequestration— Moving Carbon from the Atmosphere to the Lithosphere, in the 42nd Annual Meeting of the North-Central Section of the Geological Society of Americ*a, April 2-3, 2009, Rockford, Illinois, USA.

C20. **Quanlin Zhou**, Jens T. Birkholzer, Chin-Fu Tsang, Hannes Leetaru, Edward Mehnert, Keni Zhang, Preston Jordan, Scott Frailey, and Robert Finley, 2008. Modeling of basin-scale pressure perturbations induced by geological carbon sequestration in a sedimentary basin, *the Virtual Conference on Climate Change and CO_2 Storage*, December 3rd, 2008, Imperial College, London.

C21. Monica Gasca, Theodore Johnson , Sally McCraven , **Quanlin Zhou** , Julio Garcia, 2008. Natural photolysis and biodegradation of NDMA at groundwater recharge facilities that use recycled water, Los Angeles County, California, *The 21st Symposium of Groundwater Resources Association of California on Emerging Contaminants 2008*, San Jose, CA, November 19-20, 2008.

C22. Hannes Leetaru, Scott Frailey, James Damico, Edward Mehnert, Jens Birkholzer, **Quanlin Zhou**, and Preston Jordan, 2008. Understanding CO_2 plume behavior during sequestration projects through the use of reservoir fluid modeling, *9th International Conference on Greenhouse Gas Technologies*, Washington DC, November 16-20, 2008.

C23. **Quanlin Zhou**, Jens T. Birkholzer, Chin-Fu Tsang, 2008. Environmental impact of large-scale CO_2 injection and storage in a multi-sequence aquifer-seal system: pressure propagation and brine displacement, *The Seventh Annual Conference on Carbon Capture & Sequestration*, Pittsburgh, PA, May 5-8, 2008.

C24. Sally McCraven, Phyllis Stanin, **Quanlin Zhou**, 2008 (Talk). Occurrence, fate, and transport of N-Nitrosodimethylamine (NDMA) in California Groundwater, *Sixth International Conference on Remediation of Chlorinated and Recalcitrant Compounds*, Monterey, CA, May 19-22, 2008.

C25. Sally McCraven, **Quanlin Zhou**, Julio Garcia, Monica Gasca, and Ted Johnson, 2008 (Talk). Characterizing field biodegradation of N-Nitrosodimethylamine (NDMA) in groundwater near reclaimed water recharge areas, *Annual California WateReuse Conference*, Newport Beach, CA, March 24-26, 2008.

C26. **Quanlin Zhou**, Jens Birkholzer, Jonny Rutqvist, and Chin-Fu Tsang, 2007 (Talk). Sensitivity study of CO_2 storage capacity in brine aquifers with closed boundaries: Dependence on hydrogeologic properties, *Sixth Annual Conference on Carbon Capture & Sequestration*, Pittsburgh, PA, May 7-10, 2007.

C27. Jacob Bensabat, Jacob Bear, and **Quanlin Zhou**, 2006. Large scale modeling of seawater intrusion in a coastal aquifer: Application to the North Sharon and Heffer Valley areas, Israel, *CMWR XVI - Computational Methods in Water Resources, XVI International Conference*, Copenhagen, Denmark, June 19-22, 2006.

C28. **Quanlin Zhou**, 2006. Validation of the active fracture model for unsaturated fracture flow using numerical experiments, in *Proceedings of TOUGH Symposium 2006*, Berkeley, CA, May 15-17, 2006.

C29. **Quanlin Zhou**, Jens T. Birkholzer, Iraj Javandel, and Preston D. Jordan, 2003. Simulation of groundwater flow at the LBNL site using TOUGH2, in *Proceedings of TOUGH Symposium 2003*, Berkeley, California, May 12-14, 2003.

C30. **Quanlin Zhou**, Gudmundur S. Bodvarsson, Hui-Hai Liu, and Curtis M. Oldenburg, 2002 (Talk). Characterization of spatial variability of hydrogeologic properties for the unsaturated flow in the fractured rocks at Yucca Mountain, Nevada, in *Proceedings of the International Groundwater Symposium on Bridging the Gap between Measurements and Modeling in Heterogeneous Media*, Berkeley, California, March 25-29, 2002.

C31. **Quanlin Zhou**, Lynn W. Gelhar, and Bruce Jacobs, 2002 (Talk). Comparison of the field-scale effective properties of two-phase flow in heterogeneous porous media obtained by stochastic analysis and numerical experiments, in *Proceedings of the International Groundwater Symposium* *on Bridging the Gap between Measurements and Modeling in Heterogeneous Media*, Berkeley, California, March 25-29, 2002.

C32. Jacob Bear, **Quanlin Zhou**, and Jacob Bensabat, 2001 (Talk). Three-dimensional simulation of seawater intrusion in heterogeneous aquifers: Application to the coastal aquifer of Israel, in *Proceedings of the First International Conference on Saltwater Intrusion and Coastal Aquifers-Monitoring, Modeling, and Management*, Essaouira, Morocco, April 23-25, 2001.

C33. **Quanlin Zhou**, and Yuansheng Zhu, 1993 (Talk). Composite risk analysis for levee of flood plains, in *Proceedings of South and East Asia Regional Symposium on Tropic Storms and Related Flood*, 139-146, Guangzhou, China, November 22-25, 1993.

6.4 Presentations with Abstracts in Conferences and Professional Meetings

1. Birkholzer J.T., and **Zhou Q.**, 2010 (Invited Talk). On Regional Pressure Buildup and Fluid Migration in Response to Large CO2 Injection Operations, Abstract in Proceedings to 2010 GSA Annual Meeting, Denver, Colorado, October 31 to November 3, 2010.

2. Cihan A., Illangasekare T.H., **Zhou Q.**, Birkholzer J.T., and Rodriguez D., 2010. Intermediate-scale investigation of capillary and dissolution trapping during CO2 injection and post-injection in heterogeneous geologic formations, Abstract in Proceedings AGU Fall Meeting 2010, San Francisco, CA, December, 2010.

3. **Zhou Q.**, and Birkholzer J.T., 2010 (Talk). The Role of Fault Zones in Capillary and Dissolution Trapping of CO2 in the Southern San Joaquin Basin, California, Abstract in Proceedings to AGU Fall Meeting 2010, San Francisco, CA, December, 2010.

4. **Quanlin Zhou**, Fred J. Molz, Hui-Hai Liu, and Yingqi Zhang, 2008 (Talk). Scaling behavior of field-scale diffusive transport in fractured rock and porous media: A contradiction? *EOS Trans. AGU* 89(53), Fall Meet. Suppl. Abstract H31K-04, December 15-19, San Francisco, CA.

5. Jens T. Birkholzer, **Quanlin Zhou**, Preston Jordan, Chin-Fu Tsang, Hannes Leetaru, Edward Mehnert, Scott Frailey, and Robert Finley, 2008 (Talk). A hypothetical scenario for full-scale deployment of geological carbon sequestration: Investigating the interaction between multiple CO_2 storage sites in a sedimentary basin, *EOS Trans. AGU* 89(53), Fall Meet. Suppl. Abstract H12C-02, December 15-19, San Francisco, CA.

6. **Quanlin Zhou**, Jens Birkholzer, Chin-Fu Tsang, Jonny Rutqvist , 2007. Quick assessment of CO_2 storage capacity in pressure-constrained saline aquifers with different hydrogeologic properties. H13F-1662, AGU Fall Meeting, December 10-14, San Francisco, CA

7. Chin-Fu Tsang, Jens Birkholzer, **Quanlin Zhou**, 2007. Pressure propagation and brine displacement in CO_2 storage formations: The role of sealing units. H13F-1661, AGU Fall Meeting, December 10-14, San Francisco, CA.

8. Sally McCraven, **Quanlin Zhou**, Julio Garcia, Monica Gasca, and Ted Johnson, 2007. Characterizing field biodegradation of N-nitrosodimethylamine (NDMA) in groundwater with active recycled water recharge. H33E-1696, AGU Fall Meeting, December 10-14, 2007, San Francisco, CA.

9. Yingqi Zhang, Hui-Hai Liu, Stefan Finsterle, and **Quanlin Zhou**, 2005. How dual-scale diffusive property heterogeneity affects the effective matrix diffusion coefficient in fractured rock. AGU Fall Meeting, December 5-9, 2005, San Francisco, CA

10. **Quanlin Zhou**, Jens T. Birkholzer, Iraj Javandel, and Preston D. Jordan, 2004. Refining a three-dimensional groundwater flow model at a heterogeneous site in support of remediation. H11C-0316, AGU Fall Meeting, December 13–17, 2004, San Francisco, CA.
11. **Quanlin Zhou**, Gudmundur S. Bodvarsson, Hui-Hai Liu, and Curtis M. Oldenburg, 2001. Calibration of spatial variability of hydrogeologic properties in the unsaturated fractured rock at Yucca Mountain, Nevada. H31C-0259, AGU Fall Meeting, December 10–14, 2001, San Francisco, CA.

6.5 Seminars by Quanlin Zhou

1. Science and Technology Challenges in Geologic Carbon Sequestration (GCS): Storage Capacity, Heterogeneity Effects, and Monitoring and Leakage Detection, at Beijing Normal University, Beijing, January 10, 2011.
2. Overview of Geologic Carbon Sequestration in the United States: Update and Challenges, at the Institute of Geology and Geophysics, China Academy of Sciences, Beijing, January 5, 2011
3. TOUGH2 Modeling for Geologic Carbon Sequestration: Fundamentals and Application to the Southern San Joaquin Basin, California, at the Institute of Geology and Geophysics, China Academy of Sciences, Beijing, January 5, 2011.
4. Data Analysis of the Frio Brine Pilot Tests: Characterizing Multiscale Heterogeneity and Evaluating its Effects on CO2 Storage, at the Institute of Geology and Geophysics, China Academy of Sciences, Beijing, January 5, 2011.
5. Science and Technology Challenges in Geologic Carbon Sequestration (GCS): Storage Capacity, Heterogeneity Effects, and Monitoring and Leakage Detection, at China University of Geosciences, Beijing, January 4, 2011.
6. Modeling Geologic Carbon Sequestration (GCS) and Some Thoughts on Pressure-Driven Geomechanical Processes, at the Geotechnical Institute, Hohai University, Nanjing, China, October 15, 2009.
7. Climate Change and U.S. Energy Research: The Role of Carbon Capture and Sequestration, at the Research Center for Climate Change, the Ministry of Water Resources, Nanjing Hydraulic Research Institute, Nanjing, China, October 14, 2009.
8. Climate Change and U.S. Energy Research: The Role of Carbon Capture and Sequestration, at the Key State Laboratory of Water Resources and Hydraulic Engineering, Hohai University, Nanjing, China, October 13, 2009.
9. Geologic Carbon Sequestration (GCS) in the Illinois Basin: From Site Characterization to Full-Scale Deployment, at the Institute of Geology and Geophysics, China Academy of Sciences, Beijing, China, September 29, 2009.
10. Geologic Carbon Sequestration (GCS) in the Illinois Basin: From Site Characterization to Full-Scale Deployment, at the Institute of Rock and Soil Mechanics, China Academy of Sciences, Wuhan, China, September 22, 2009.
11. Numerical investigation of multiphase flow and transport in heterogeneous porous and fractured media, at Lawrence Livermore National Laboratory, April 2002.
12. Numerical investigation of field-scale effective properties of two-phase flow in heterogeneous porous media, at Lawrence Berkeley National Laboratory, September 2001.

13. Numerical investigation of effective properties of multiphase flow in heterogeneous porous media, at Massachusetts Institute of Technology, September 2000.
14. Modeling of strongly density-dependent flow and transport problems, at Massachusetts Institute of Technology, April 2000.
15. Modeling of strongly density-dependent flow and transport problems, at the University of Texas at Austin, March 2000.
16. Modeling seawater intrusion in coastal aquifers, at the Technion-Israel Institute of Technology, Haifa, Israel, June 1999.

7. STATEMENT OF RESEARCH

During my tenure at LBNL from March 2001 to the present, I have been working on (1) geologic carbon sequestration projects for mitigating global climate change, (2) the Yucca Mountain project for characterizing the geologic repository site for nuclear waste disposal, and (3) site-specific contamination remediation and assessment projects. My research at LBNL focuses on the following four areas.

1. Analytical and Numerical Modeling of Geologic Carbon Sequestration (GCS) [J1–J6, J8–J10]

In order to make GCS an effective measure for climate change mitigation, we face three grand challenges: (1) subsurface storage capacity is constrained by pressure buildup and its adverse effects (e.g., caprock integrity damage, induced seismicity, and fault reactivation); (2) the effects of subsurface heterogeneity on CO_2 migration, long-term trapping, and storage efficiency need to be better quantified; and (3) monitoring and joint inversion methods for early warning and detection of CO_2 leakage need development. In the past five years, I focused my research on (1), via analytical and numerical modeling.

My research in the area of high-performance, numerical modeling of CO_2-brine flow and single-phase brine flow focuses on (1) understanding pressure buildup and brine migration induced by GCS in closed, semi-closed, and open sedimentary basins with simplified systems [J9, J10], (2) evaluating the dynamic storage capacity and impact of GCS on groundwater resources in the Illinois Basin and the southern San Joaquin Basin, as examples, to understand the full-scale deployment and pressure-constrained dynamic storage capacity under operation [J3, J5, J6], and (3) assessing brine leakage through abandoned wells, including nonisothermal effects [J2]. My research shows the limiting effect of pressure buildup on dynamic storage capacity to avoid adverse geomechanical and environmental effects, although the constraint is moderated by pressure propagation in the storage formation and pressure bleed-off into overlying/underlying formations. The secondary-seal effect was manifested by retarding upward CO_2 migration through multiple secondary (more permeable) seals, coupled with lateral CO_2 viscous fingering through high-permeability layers [J5, J6].

My research also includes development and application of new analytical solutions to single-phase brine flow: (1) a solution developed for pressure perturbations and leakage in a laterally bounded aquifer-aquitard system, complementing the solutions for infinite systems developed by Theis, Hantush, Neuman, and Moench [J4, J8], and (2) a solution developed for pressure perturbations and leakage through aquitards and leaky abandoned wells in a multilayered system, generalizing well hydraulics to a system of any number of aquifers, alternative semi-pervious aquitards, injection wells, and leaky wells [J1]. The super-computational efficiency of these solutions facilitates analyzing the sensitivity of pressure buildup and brine-flow rate to hydrogeologic properties of storage formation, seals, and leaky structures, developing pressure management schemes using inverse modeling, and providing insights into leakage detection using pressure data.

2. Field-Scale Diffusive Transport in Fractured and Porous Media [J11, J13–J16]

Diffusive transport has been demonstrated to be one of the key transport phenomena in fractured rock, through mathematical modeling, laboratory experiments, and field tracer tests. However, its behavior in the field is more complicated because of the interplay of advection and dispersion in fracture networks with diffusion in the rock matrix of naturally heterogeneous systems. Along with other colleagues, I have proposed and systematically demonstrated that the field-scale, effective matrix diffusion coefficient for heterogeneous fractured rock might be dependent on the observation scale, following the findings of scale-dependent hydraulic conductivity and macrodispersivity. This conclusion was based on our studies of a critical literature review, numerical experiments, and tracer-test analyses: (1) a comprehensive critical review was conducted for all field-scale tracer tests in the literature, showing that the field-scale, effective matrix diffusion coefficient is scale-dependent [J13]; (2) numerical experimental results indicate scale-dependent behavior, with a slope dependent on the local matrix diffusion coefficient, aperture ratios between different levels of fractures, and the scaling feature for the network of multiscale (length, aperture) fractures [J14]; (3) numerical experiments indicate that the spatial variability of the local-scale matrix diffusion coefficient along single or multiple parallel flow paths does not contribute to the observed scale-dependent behavior [J15]; (4) modeling analysis of a long-term field-scale tracer test shows spatial variability of the local-scale matrix diffusion coefficient within the rock matrix in the direction perpendicular to the fracture-matrix wall [J16]. This scale-dependent behavior stems from the heterogeneous network of multiscale fractures, rather than the spatial variability in the local-scale matrix diffusion coefficient. This observation may have strong implications with respect to enhanced solute or radionuclide retardation in fractured rock.

In contrast to our observations regarding fractured rock, Haggerty et al. [2004] found that the mass-transfer rate coefficient in porous media decreases with experimental duration or residence time, using analyses of 316 transport experiments. Following the analyses of numerous experiments using the first-order mass-transfer model, we analyzed the MADE-2 tracer test and concluded that the field-scale mass-transfer rate coefficient decreases over tracer residence time. However, we challenged Haggerty et al.'s [2004] conclusions, finding that this scale-dependent behavior is mainly an artifact of numerical model approximations, rather than the real physical process of multirate diffusion [J11].

3. Flow and Transport in Heterogeneous Fractured/Porous Media [J7, J12, J17– J20]

I have focused my research on a broader area of flow and transport in heterogeneous, saturated/unsaturated fractured/porous media. This research has included (1) characterization of multiscale heterogeneity of hydrogeologic properties in the fractured unsaturated zone at Yucca Mountain, and prediction of unsaturated flow and solute transport in heterogeneous fractured rock [J20]; (2) analysis of a mesoscale infiltration and seepage test and correlation between infiltration/seepage rates and mapped fractured patterns through modeling and field observations [J17]; (3) development of a density-dependent flow simulator and application of it to saltwater upconing and decay beneath a well pumping [J18]; (4) calibration of saturated groundwater flow at a DNAPL-contaminated site (in support of on-site remediation) [J19]; and (5) discovery of field evidence for significant *in situ* biodegradation of N-Nitrosodimethylamine (NDMA), through field monitoring and numerical modeling of a large-scale groundwater system receiving recycled water as incidental and active recharge [J7].

4. Subsurface Heterogeneity Tomography and Early Warning and Detection of CO_2 Leakage

With five ongoing projects and support from four postdocs, I am developing two new research interests. My first new research interest is the investigation of CO_2 migration, long-term trapping, and storage efficiency in hierarchical, multiscale heterogeneous sedimentary rock, and the development of the methodology of subsurface heterogeneity tomography (SHT) (Challenge 2). I developed conceptual models for a number of key transport processes in heterogeneous formations: (1) viscous fingering of free-phase CO_2 along high-permeability (or high-K) fast-flow pathways; (2) dynamic intrusion of CO_2 from high-K zones into relatively low-K zones by capillarity and buoyancy; (3) diffusive transport of dissolved CO_2 into low-K zones across large interface areas created by CO_2 fingers; and (4) density-driven convective mass transfer into CO_2-free regions confined by shale layers. These CO_2 migration and trapping processes are investigated at core scale (centimeters, working with a partner in China), at laboratory scale (1–5 m), at field pilot scale at the Frio site (~100 m), and at large storage scale at Kevin Dome, Montana (kilometers). In addition, the SHT methodology will be developed using hydraulic-thermal-tracer-CO_2 storage tests in the field, borehole logs, and other raw hydrogeologic data. SHT will be tested and applied to the Frio Pilot Test, a small-scale CO_2 storage experiment that offers a wealth of diverse monitoring data for hydraulic, thermal, tracer, and CO_2 injection tests.

My second new research interest involves early warning and detection of CO_2 leakage through seal imperfections (e.g., fractures, abandoned wells, and fault zones) by real-time monitoring of fast-propagating pressure and ground-surface uplift at a large scale and of slow-migrating CO_2 plume at the plume scale, and by deterministic and stochastic joint inversion (Challenge 3). The key to early leakage detection is to detect pressure-driven brine leakage through leakage pathways as early as possible, to predict the relatively slow CO_2 plume migration in the storage reservoir for CO_2 leakage, and to guide deployment of monitoring for improving data and detection, with the ultimate goal of mitigating leakage risks. This new technology is under development—it will be tested and applied to the CO_2 injection and storage at the Ketzin, Germany site, and at the In Salah, Algeria site, with sufficient data and potential fault leakage of CO_2/brine.

8. RESEARCH SUMMARY

During my stay at LBNL from March 2001, I have been working on (1) geologic carbon sequestration (GCS) projects for mitigating global climate change, (2) the DOE's Yucca Mountain Project for characterizing Yucca Mountain, Nevada, as the first geologic repository site for high-level nuclear waste disposal, and (3) site-specific contamination remediation and assessment projects.

8.1 Research Highlights

8.1.1. Geological Carbon Sequestration

I have been working on eight research projects in the area of geologic carbon sequestration since 2006. I have been PI or Co-PI for six projects funded by DOE, EPA, LBNL, and California Energy Commission (CEC), with a total fund of $10.0M. In particular, I am co-leading a long-term, $5.6M project on modeling and monitoring support of the Big Sky Partnership's Phase III project at Kevin Dome (FY2011 – FY2018). I have been focusing my research in the following four areas:

- Physical processes and phenomena at sedimentary basin scale and large-scale impacts: Dynamic pressure buildup and brine migration in storage formations and overlying/underlying formations; natural attenuation of pressure buildup through semi-pervious sealing units and seal imperfections (e.g., abandoned wells and fault zones) in multilayered systems; dynamic storage capacity in pressure-constrained systems with natural pressure attenuation and pressure management; site-specific evaluation of the large-scale impact in the Illinois Basin, IL, and the San Joaquin Basin (Kimberlina site), CA, where DOE's Phase III demonstration projects are under way *[J1–J6, J8–J10]*. The research projects include the 6-year DOE project on large-scale hydrologic impact and the CEC project on the impact of GCS on groundwater resources in California's Central Valley.
- Physical processes and transport phenomena at CO_2 plume scale and enhanced storage efficiency and safety: Effects of hierarchical, multiscale heterogeneity on CO_2 migration and trapping in sedimentary rock; enhanced CO_2 trapping by (1) capillary intrusion into numerous low-permeability lenses from viscous, mobile CO_2 fingers in sand channels and (2) diffusive transport and density-driven fingering of dissolved CO_2 within sand channels and into low-permeability layers and lenses; improved storage safety by enhanced capillary and dissolution trapping in heterogeneous formations *[J5]*. The research projects includes the LDRD project on characterization of multiscale heterogeneity through field hydraulic-thermal-tracer-CO_2 testing and monitoring at the Frio Pilot site, and the DOE project on intermediate-scale laboratory experiments. Ongoing research includes investigating the effect of heterogeneity on CO_2 migration and trapping at core scale (centimeters, working with a China partner), laboratory scale (1-5 m), field pilot scale at the Frio site (~100 m), and large storage scale at Kevin Dome, Montana (kilometers scale).
- Early warning and detection of CO_2/brine leakage using inverse modeling and the signals of fast-propagating pressure and pressure-driven processes (e.g., ground surface uplift); the concept of early leakage detection is to detect pressure-driven brine leakage through leakage pathways as early as possible, to predict the relatively slow CO_2 plume migration in the storage reservoir for

CO_2 leakage, and to guide deployment of monitoring for improving data and detection, with the ultimate goal for mitigating leakage risks. This new technology and methodology is under development, with $2.0M support from a 5-year DOE's research project. The technology will be applied to the CO_2 injection and storage at the Ketzin, Germany site, and the In Salah, Algeria site with sufficient data and potential fault leakage.

- Evaluation of the EPA Area-of-Review (i.e., Area of Potential Influence) and leakage through abandoned wells using analytical and numerical modeling of multilayered sedimentary basins for pressure buildup, brine displacement, and CO_2 plume; collaborative work with EPA has been secured, and new generalized analytical solutions for coupled diffuse leakage through seals and focused leakage through leaky wells have been developed *[J1–J2, J5–J6, J8–J10]*. The research is funded by EPA.

8.1.2. Nuclear Waste Disposal and Transport in Fractured Rocks

I worked on the Yucca Mountain Project on the study of flow and transport in the unsaturated fractured rock from 2001 to 2006, and focused my research on:

- Scale dependence of the field-scale, effective matrix diffusion coefficient in fractured media, enhanced retardation of solute/radionuclide transport by diffusive mass transfer between fractures and the matrix in heterogeneous fractured rock, and scale dependence of the mass transfer coefficient in porous media [J11, J13–J16];
- Effects of flow focusing in unsaturated, heterogeneous fractured rock on total system performance assessment, and calibration of unsaturated zone properties [C27];
- Pretest prediction and analysis of the Alcove 8–Niche 3 field infiltration/seepage and tracer tests (conducted at mesoscale in two tunnels), and understanding of observed spatial variability of infiltration/seepage rates and mapped fracture patterns [J17];
- Effects of multiscale heterogeneity in fracture/matrix permeability and capillarity on unsaturated flow and radionuclide transport—by characterizing and calibrating the spatial variability of fracture and matrix properties at multiple scales [J20].

8.1.3. Site-Specific Contaminant Remediation and Assessment

I have been involved in four individual projects related to site-specific contamination remediation and assessment. Through detailed data analysis and model calibration, I have been devoted to physically-based remediation measures and in-situ biodegradation evidenced from detailed monitoring data. Specifically, I have focused my research on:

- Development and calibration of a three-dimensional numerical model for modeling groundwater flow and advective transport at the DNAPL-contaminated LBNL site in support of the ongoing remediation process: hydraulic control of dissolved DNAPL plumes [J19];
- Photo- and biodegradation of N-nitrosodimethylamine (NDMA) in a coupled surface water and groundwater system with active recycled water recharge in Montebello Forebay, Los Angeles, California. Evidence of in-situ biodegradation in saturated groundwater was, for the first time, obtained through detailed monitoring, data analysis, and modeling. This research is of significance to water supply in the Los Angeles Metropolitan with expanded artificial recharge [J7];

- Transport of tritium in the NuMI underground facility at FermiLab, IL, where tritium was generated in concrete shielding, fractured rock, steel, and vapor by accelerator experiments. Key components and processes are global transport of tritiated water vapor through the tunnel, diffusive deposition into unsaturated concrete and rock in contact with the tunnel, and diffusive tritium transport within concrete and steel. This is an excellent case for investigation of multiphase diffusive transport phenomena;
- Modeling of DNAPL migration and dissolved component transport in a weathered, fractured rock zone at a contaminated site in Charlotte, North Carolina, in support of full-scale remediation; evidence of back diffusion from the matrix to fractures in response to remediation of a long-term TCE plume.

8.1.4. Seawater Intrusion and Multiphase Flow Modeling

In 2000, my postdoctoral research at MIT was on multiphase flow simulation and effects of heterogeneity on multiphase flow (effective properties and DNAPL lateral spreading). The effective properties of multiphase flow obtained by numerical simulation were compared with those obtained by spectral-perturbation analysis, and a reasonable agreement was obtained. My PhD research (1996–1999) at Technion was on modeling seawater intrusion in coastal aquifers, with applications to seawater intrusion in the coastal aquifer of Israel. In China (1990–1996), I was engaged in research on surface water modeling, water resources systems analysis, and risk and uncertainty analysis.

During the time I have worked on projects related to DOE's missions for geologic waste disposal and containment and remediation, I have developed my scientific research capabilities in three major categories: (1) analytical and numerical modeling of geologic carbon sequestration, (2) diffusive transport phenomena in fractured and porous media at field scale, and (3) flow and transport in heterogeneous fractured/porous media under single- and multiphase flow conditions.

8.2. Analytic and Numerical Modeling of Geologic Carbon Sequestration [J1–J6, J8–J10]

Geologic carbon sequestration (GCS) has been investigated for more than two decades, from early concept studies in the late 1980's to field pilot tests, and to a limited number of industrial-scale applications. In order for GCS to be an effective measure for climate change mitigation, we are facing three grand challenges: the storage capacity of the subsurface is constrained by pressure buildup and its adverse effects (e.g., caprock integrity damage, induced seismicity, and fault reactivation); effects of subsurface heterogeneity on CO_2 migration, long-term trapping, and storage efficiency need to be better quantified; and monitoring methods for early warning and detection of CO_2 leakage need improvement. I have been working on GCS for five years, focusing my research on the large-scale impact of CO_2 storage on groundwater resources in shallow aquifers, including pressure propagation and brine displacement (Challenge 1). Meanwhile, with several ongoing projects, I am developing research in (1) enhanced storage efficiency and safety in hierarchical, multiscale heterogeneous sedimentary rock (Challenge 2), and (2) early warning and detection of CO_2 leakage through sealing unit imperfections (e.g., fractures, abandoned wells, and fault zones) by real-time monitoring of pressure, ground-surface uplift at the large scale and of CO_2 plume at the plume scale, and deterministic and stochastic joint inversion (Challenge 3).

Nine journal publications in GCS present my research on pressure propagation and brine displacement within the storage formation and from the storage formation to the shallowest aquifer, via diffuse leakage through permeable seals and via focused leakage through leaky, abandoned wells. Numerical modeling of multiphase flow (CO_2, water, and NaCl) and multicomponent transport is the key instrument for our understanding [J2, J3, J5, J6, J9, J10]. Hypothetical storage scenarios for full-scale deployment of GCS in the Illinois Basin and the southern San Joaquin Basin in California have been studied to answer how much we can store CO_2 underground, taking into account pressure-related caprock integrity and environmental constraints. The highlights of these journal publications in the area of numerical modeling are listed as follows:

J3. The scale and magnitude of pressure perturbation and brine migration induced by geologic carbon sequestration is discussed assuming a full-scale deployment scenario in which enough CO_2 is captured and stored to make relevant contributions to global climate change mitigation. In this scenario, the volumetric rates and cumulative volumes of CO_2 injection would be comparable to or higher than those related to existing deep-subsurface injection and extraction activities, such as oil production. Large-scale pressure build-up in response to the injection may limit the dynamic storage capacity of suitable formations, because over-pressurization may fracture the caprock, may drive CO_2/brine leakage through localized pathways, and may cause induced seismicity. On the other hand, laterally extensive sedimentary basins may be less affected by such limitations because (i) local pressure effects are moderated by pressure propagation and brine displacement into regions far away from the CO_2 storage domain; and (ii) diffuse and/or localized brine migration into overlying and underlying formations allows for pressure bleed-off in the vertical direction. A quick analytical estimate of the extent of pressure build-up induced by industrial-scale CO_2 storage projects is presented. Also discussed are pressure perturbation and attenuation effects simulated for two representative sedimentary basins in the USA: the laterally extensive Illinois Basin and the partially compartmentalized southern San Joaquin Basin in California. These studies show that the limiting effect of pressure build-up on dynamic storage capacity is not as significant as suggested by Ehlig-Economides and Economides, who considered closed systems without any attenuation effects.

J2. This paper discusses the potential for brine leakage to occur in temperature-and salinity-stratified systems. Using static mass-balance calculations as well as dynamic well flow simulations, we evaluate the minimum reservoir pressure that would generate continuous migration of brine up a leaking wellbore into a fresh water aquifer. Since the brine invading the well is denser than the initial fluid in the wellbore, continuous flow only occurs if the pressure perturbation in the reservoir is large enough to overcome the increased fluid column weight after full invasion of brine into the well. If the threshold pressure is exceeded, brine flow rates are dependent on various hydraulic (and other) properties, in particular the effective permeability of the wellbore and the magnitude of pressure increase. If brine flow occurs outside of the well casing, e.g., in a permeable fracture zone between the well cement and the formation, the fluid/solute transfer between the migrating fluid and the surrounding rock units can strongly retard brine flow. At the same time, the threshold pressure for continuous flow to occur decreases compared to a case with no fluid/solute transfer.

J5. As an example, an integrated modeling of basin- and plume-scale transport processes for a scenario of full-scale deployment of GCS in the Illinois Basin was conducted, on the basis of detailed site characterization. Twenty storage sites, located in the central most suitable area, referred to as core injection area, of 24,000 km^2, were employed with annual injection rate of 5 million metric tonnes CO_2 per site over 50 years. The storage rate accounts for one third of the current CO_2 emissions in the region. Significant pressure buildup (as high as 35 bar) was observed in the core injection area and moderate pressure buildup is propagated to the margin of the Illinois Basin of 240,000 km^2.

Various conditions in the selected core injection area are favorable to the large-scale deployment of GCS, as shown by simulated CO_2 plumes consisting of a typical gravityoverride subplume in the bottom injection zone of high injectivity and a pyramid-shaped subplume in the overlying multilayered Mt. Simon, indicating the important role of a secondary seal with relatively low-permeability and high-entry capillary pressure. The secondary-seal effect is manifested by retarded upward CO_2 migration as a result of multiple secondary seals, coupled with lateral preferential CO_2 viscous fingering through high-permeability layers.

J6. On the basis of the integrated modeling of GCS the Illinois Basin, the implications of the model results to dynamic storage capacity assessment and GCS regulation were discussed. Any storage capacity assessment has to base on detailed modeling with site-specific pore compressibility and preliminarily designed storage scenario for the ultimate deployment; the methodology based on pore space available may overestimate storage capacity, in particular for low pore compressibility sandstones.

J9. Large volumes of CO_2 captured from carbon emitters such as coal-fired power plants may be stored in deep saline aquifers as a means of mitigating climate change. Storing these additional fluids may cause pressure changes and displacement of native brines, affecting subsurface volumes that can be significantly larger than the CO_2 plume itself. Serious environmental impacts on groundwater resources may result if the deep parts of the basin communicate effectively with shallow units. One concern is the large-scale pressure perturbation within a storage formation that may extend updip to a shallow freshwater aquifer or recharge/discharge zones. Another would be the slow pressure propagation in the vertical direction, limited but possibly not inhibited by the sealing formations that separate deep and shallow units. In an attempt to address these issues quantitatively, we have conducted numerical simulations that provide a basic understanding of the large-scale flow and pressure conditions in response to industrial-scale CO_2 injection into a laterally open saline aquifer. The model domain includes an idealized multilayer groundwater system, with a sequence of aquifers and aquitards (sealing layers) extending from the deep saline storage formation to the top of the uppermost aquifer. Simulation results show the region of influence during/after injection of CO_2 in both lateral and vertical directions. For seal permeability higher than 0.01 mDarcy, pressure buildup of at least 1.0 m occurs in the shallow groundwater aquifer. With seal permeability of 0.001 mDarcy (representative of a number of CO_2 storage or test sites), interlayer communication through low-permeability seals significantly reduces the pressure buildup in the storage formation, avoiding geomechanical damage of the sealing units.

J10. Carbon dioxide may be stored in compartmentalized closed and semi-closed systems with no-flow radial boundaries, with the benefit of low CO_2 leakage risks. However, the pressure buildup caused by continuous industrial-scale CO_2 injection may have a limiting effect on CO_2 storage capacity. The storage capacity and pressure buildup in these systems were investigated using numerical simulations. An analytic solution was developed for the quick assessment of the CO_2 storage capacity. This quick-assessment method is based on the fact that native brine (of an equivalent volume) displaced by the cumulative injected CO_2 occupies additional pore volume within the storage formation and the seals, provided by pore and brine compressibility in response to pressure buildup. With nonideal seals, brine may also leak through the seals into overlying/underlying formations. The quick-assessment method calculates these brine displacement contributions in response to an estimated average pressure buildup in the storage reservoir. The developed solution can be used as a screening tool for site selection.

Analytic solutions to single-phase brine flow are also developed for a laterally bounded aquifer-aquitard system, complementing the solutions for infinite systems developed by Theis, Hantush, Neuman, and Moench, and for a multilayered system with any number of injection and leaky wells, generalizing the well hydraulics [J1, J4, J8]. These solutions can be applied to simplified systems with super computational efficiency, so that they are useful to understand the sensitivity of system responses (pressure buildup and brine flow rate) to hydrogeologic properties of the storage formation, seals, and the leaky structures.

J1. Generalized analytical solutions were developed to account for the combined effect of diffuse leakage through permeable aquitards and of focused leakage through leaky, abandoned wells. The new solutions solve for pressure changes in a system of N aquifers with alternating leaky aquitards in response to fluid injection/extraction with any number, NI, of injection/pumping (active) wells, and passive leakage/recharge in any number, NL, of leaky wells. The equations of horizontal groundwater flow in the aquifers are coupled by the vertical flow equations in the aquitards and by the flow continuity equations in the leaky wells. The solution methodology involves transforming the transient flow equations into the Laplace domain, decoupling the resulting ordinary differential equations (ODEs) coupled by diffuse leakage via Eigenvalue analysis, solving a system of NL × N linear algebraic equations for the unknown rates of flow through leakage wells, and superposing the solution of pressure buildup/drawdown in aquifers and aquitards resulting from flow in the NI active and NL leaky wells. Verification of the new solutions was achieved by comparison against existing analytical solutions for diffuse leakage and for focused leakage, and against a numerical solution for combined diffuse and focused leakage. Application to an eight-aquifer system with leaky aquitards and one leaky well demonstrates the usefulness and efficiency of the approach, and illustrates the pressure behavior over a spectrum of leakage scenarios and parameters.

J8. We developed semi-analytical solutions to address the injection/storage-induced pressure perturbation and vertical leakage in a "laterally bounded" system. A one-dimensional radial-flow equation for the aquifer was coupled with a one-dimensional vertical-flow equation for the aquitards. Analytical solutions in the Laplace-transform domain were obtained for (1) pressure change in the aquifer and in the underlying/overlying aquitards, (2) rate and volume of leakage through the aquifer-aquitard interface integrated up to an arbitrary radial distance, (3) total leakage rate and volume for the entire interface, and (4) integrated horizontal flux at an arbitrary radius. The derived analytic solutions for bounded systems are the generalized solutions of infinite systems, with an extra term reflecting the effect of the no-flow boundary. In addition, it was mathematically proven that the total leakage rate and volume are independent of the aquifer's radial extent and wellbore radius, a scale invariant, self-adjusting phenomenon. Laplace-transform solutions were numerically inverted to obtain the pressure change, leakage rate, and leakage volume for the given hydrogeologic and geometric conditions of the aquifer-aquitard system.

8.3. Diffusive Transport Phenomena in Fractured and Porous Media [J11, J13–J16]

Since matrix diffusion was employed to interpret a groundwater tritium anomaly observed in the field [Foster, 1975], diffusive transport has been demonstrated to be one of the key transport phenomena in fractured rock, as reflected in mathematical modeling, laboratory experiments, and field tracer tests. For heterogeneous fractured rock and porous media, two different types of scale-dependence behavior for the field-scale, effective matrix diffusion coefficient or mass-transfer rate coefficient have been suggested, following the findings of scale-dependent hydraulic conductivity and macrodispersivity.

The first scaling behavior, proposed by our research group, is that the field-scale, effective matrix diffusion coefficient (D_m^e) increases with observation scale (L), indicating a transport mechanism for enhanced retardation of solute/radionuclide in fractured rock. The scaling factor (F_D) of the effective matrix diffusion coefficient is defined as the ratio of D_m^e to the geometric mean (D_m^G) of local-scale matrix diffusion coefficient (D_m), and the scaling slope of $\log_{10}(F_D)$ as a function of $\log_{10}(L)$ is used to describe this scaling behavior. To confirm the proposed scale dependence of effective matrix diffusion coefficient, we have conducted (1) a comprehensive and critical literature survey, (2) numerical experiments, and (3) field tracer test analyses, as summarized in my Journal Publications J13 through J16 in the Journal Publication List:

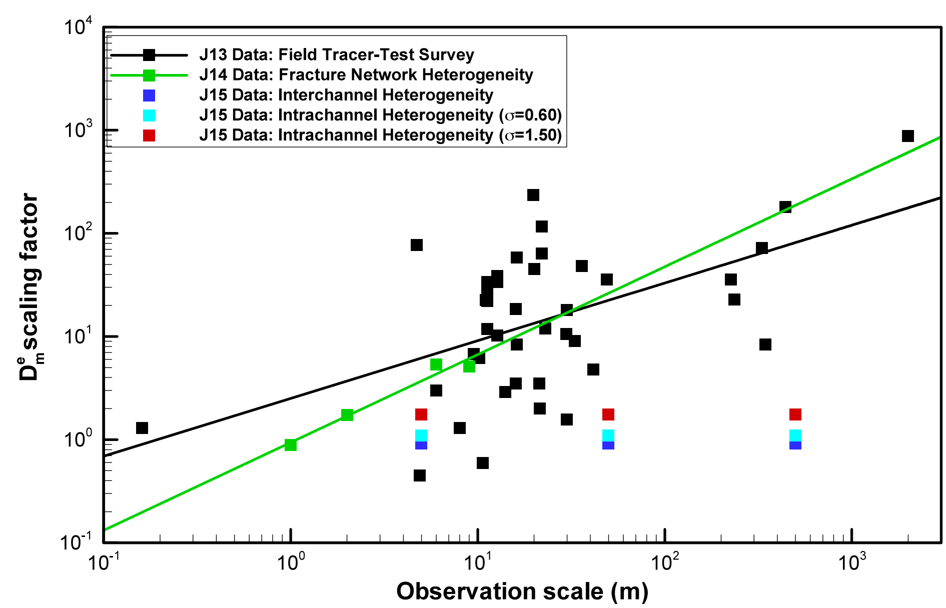
J13. We have conducted a critical review of all field-scale tracer tests available in the literature, selected 40 field tracer tests from 15 geologic sites, reanalyzed some of the tracer tests, and concluded that the field-scale, effective matrix diffusion coefficient is scale-dependent. The field-scale, effective matrix diffusion coefficient varies from 0.5 to 884 for the observation scale ranging from 5 to 2,000 m, with a scaling slope of 0.66. The tracer-test reanalysis was conducted using various (semi-) analytic solutions implemented in the iTOUGH2-TRAT code for inverse modeling. We also demonstrated that the field-scale dispersivity in fractured rock is scale dependent in the framework of advection-dispersion-diffusion calibration, consistent with previous findings by Gelhar and others. Various mechanisms behind the scale-dependence behavior and enhancement of matrix diffusion were suggested.

J14. One mechanism is the network of multiscale (length, aperture) fractures. We conducted numerical experiments to investigate the contribution of heterogeneity in fracture network to the observed scale dependence behavior. A combination of local, multilevel flow loops (in relatively small fractures) and a global flow path (in a backbone fracture), with some scaling features of network geometry, was used to represent a complex multiscale fracture network. Matrix diffusion was employed to represent mass transfer between fractures and the matrix. The effective diffusion coefficient was calibrated for different locations along the global flow path. Experimental results indicate that the effective matrix diffusion coefficient increases with observation scale, with a slope dependent on the local matrix diffusion coefficient, aperture ratios between different levels of fractures, and the scaling feature for the fracture network. The scaling slope can be as high as 1.0 when all favorable conditions prevail along a travel distance less than 10 m. In these numerical experiments, a constant local matrix diffusion coefficient was used. In summary, the geometry of a multiscale fracture network with the ultimate process of matrix diffusion is the key for the scale-dependent behavior of field-scale, effective matrix diffusion coefficient.

J15. The other mechanism is the spatial variability of the local-scale matrix diffusion coefficient (D_m) along the flow path within a single fracture (i.e., intrachannel heterogeneity) and among different fracture channels (i.e., interchannel heterogeneity). Numerical experiments were conducted for a fracture network of 10 separate, parallel channels, with lognormal distribution of the local matrix diffusion coefficient and water mixing only at the observation points (e.g., pumping wells) a 5, 50, and 500 m. No scale dependence of the calibrated matrix diffusion coefficient was observed, nor was any enhancement of matrix diffusion (calibrated D_m^e versus D_m^G, the geometric mean of D_m) for the interchannel heterogeneity. In the numerical experiments with intrachannel heterogeneity, it was observed that $D_m^e > D_m^G$, indicating an enhancement in matrix diffusion. An empirical estimate of D_m^e was given as a function of the variance of ln(D_m). However, no scale dependence was observed for the random fields of ln(D_m) (with negligible correlation length) used in this paper. Only when the ratio between the integral scale of ln(D_m), and the observation scale was between 0.1 and 10, could the scale dependence caused by intrachannel heterogeneity along the single-fracture flow path occur, as demonstrated by stochastic analysis in Dai et al. [2007]. However, the scaling slope for the observed scale dependence caused solely by the heterogeneity in the local matrix diffusion coefficient is very small, with the maximum scaling factor being 1.44 for 1,000 m.

J16. The other type of heterogeneity is the spatial variability of the local-scale matrix diffusion coefficient within the rock matrix in the direction perpendicular to the fracture-matrix wall. To analyze the effect of this type of heterogeneity, a unique, field-scale tracer test conducted over 600 days, with 350 days of constant-rate injection, was reanalyzed with the detailed fracture and matrix data available. Three different diffusion processes—(1) diffusion into stagnant water and infilling materials within fractures, (2) diffusion into a degraded matrix zone, and (3) further diffusion into an intact matrix zone—were evidenced from the steep rising limb, slow increasing platform, and decay-like falling limb of the concentration breakthrough curve. Different matrix diffusion coefficients were calibrated for the three zones. Short-term and long-term effects of these diffusion zones were also investigated, indicating that the thin degraded zone and within-fracture stagnant water and infilling material are critical to analysis of field-tracer tests, but their impact on long-term transport is negligible in comparison with the thick intact matrix zone.

These four publications present our understanding of the scale-dependent, field-scale effective matrix diffusion coefficient for fractured rocks (see the following Figure), complementing the understanding of other mechanisms for enhancement and scale-dependence behavior within field-scale diffusive transport (published by Neretnieks and his group, among many others, in the literature).



The second scaling behavior is shown by the mass transfer rate coefficient in porous media decreasing with experimental duration or residence time, evidenced from the analyses of numerous transport experiments by Haggerty et al. [2004]. Three causes for this scale-dependence behavior have been presented in the literature: (1) inseparable advective and diffusive transport between low-conductivity immobile and high-conductivity mobile zones, (2) inadequate characterization of the first-order mass-transfer model, and (3) multirate diffusion caused by sub-REV-scale heterogeneity. Based on 316 experiments (predominantly with the first-order model parameter available only), Haggerty et al. [2004] showed that the effective mass-transfer rate coefficient is much better correlated to the experimental/observational duration and solute residence time than velocity, and concluded that multirate diffusion might be a key cause for the scale behavior, in addition to the other two causes.

Our observations challenged Haggerty et al.'s [2004] conclusions in the following three ways:

J11. We employed the MADE-2 field tracer test, a natural gradient tracer (tritium) test, to examine the scale behavior of the mass-transfer rate coefficient, using the dual-porosity model in a three-dimensional flow and transport model. Hydraulic conductivity at mesh nodes was interpolated using a fractional Brownian motion model with detailed conductivity measurements. The mass-transfer rate coefficient was calibrated for each of the four plume snapshots at 27, 132, 224, and 328 days to obtain reasonable match between simulated and measured total mass in mobile regions and mass center locations. The calibrated mass transfer coefficient decreases from 0.5 day^{-1} at 27 and 132 days, to 0.002 day^{-1} at 224 days, and further to 0.0005 day^{-1} at 328 days, over three orders of magnitude. This observed scale-dependence behavior is similar to that of Haggerty et al. [2004], as well as others. However, unlike Haggerty et al. [2004], we interpreted the observed scale-dependence using an analytical solution for a layered system with the MADE-site-specific thickness of low- and high-conductivity zones. A constant single-rate diffusion coefficient value was used. The precisely calculated mass-transfer coefficient also decreases with time by two orders of magnitude. We concluded that the first-order mass-transfer model used in the dual-porosity model cannot capture transient concentration gradients at the interfaces between high- and low-conductivity zones, and requires a time-dependent mass-transfer coefficient to reproduce the transport processes. This scale-dependence behavior does not result from any heterogeneity or physical processes, but is an artifact of numerical approximations.

J13. We investigated the correlation between the calibrated effective matrix diffusion coefficient and experiment duration, as well as velocity, and found no correlations for the 40 tracer tests in our literature survey. This can be attributed to the contrast of hydraulic conductivity between fractures and the rock matrix being higher than four orders of magnitude, by excluding all field tracer tests in fractured porous media with smaller contrasts. Advective transport between fractures and the matrix is not the case here.

J15. No correlation between velocity and effective matrix diffusion coefficient was found in this paper for fractured rock. More importantly, the scaling effect caused by multirate diffusion with interchannel and intrachannel heterogeneity was demonstrated to be very minor, if any, in comparison with that caused by heterogeneous fracture network.

Through our five journal publications, we demonstrated that the field-scale, effective matrix diffusion coefficient for fractured rock is scale dependent, using a critical literature review, numerical experiments, and tracer-test analyses. This behavior stems from the heterogeneous network of multiscale fractures, rather than the spatial variability in the local-scale matrix diffusion coefficient. Following the analyses of numerous experiments using the first-order mass-transfer model, we analyzed the MADE-2 tracer test and concluded that the field-scale mass-transfer rate coefficient decreases over tracer residence time. However, we challenged Haggerty et al.'s [2004] conclusions, in that this scale-dependent behavior is mainly an artifact of numerical model approximations, rather than the real physical process of multirate diffusion.

8.4. Flow and Transport in Heterogeneous Fractured/Porous Media [J17, J19, J20]

In addition to my research on the scale dependence of field-scale, effective matrix diffusion coefficient in fractured rock caused by various types of heterogeneity, I have also focused on a broader research area in flow and transport in heterogeneous fractured/porous media, through (1) characterization of multiscale heterogeneity in the hydrogeologic properties of the fractured unsaturated zone, (2) analysis of a mesoscale infiltration and seepage test and correlation between infiltration/seepage rates and mapped fractured patterns, and (3) calibration of saturated groundwater flow at a DNAPL-contaminated site in support of on-site remediation.

J20. Characterization of multiscale heterogeneity in unsaturated fractured rock, and analysis of its impact on unsaturated flow and transport are important to the total system performance assessment of any geologic sites. We developed a conceptual model for the unsaturated zone of fractured rock at Yucca Mountain to represent complex heterogeneity at two scales: (1) layer scale, corresponding to geologic layering, and (2) local scale, for intralayer spatial variabilities. The layer-scale hydrogeologic properties were calibrated based on available measurements of water saturation and potential in the matrix, and pneumatic pressure in boreholes. The intralayer variabilities (by mean, variance, and correlation length) were characterized using data for each hydrogeologic layer. Random fields of matrix permeability, matrix van Genuchten α, and fracture permeability were generated, and the unsaturated flow and transport of a conservative tracer was simulated. Results show that local-scale heterogeneity has a considerable effect on unsaturated flow processes, leading to fast flow paths in both fractures and the matrix. As a result, a noticeable effect on global tracer transport is observed: early arrival of tracer mass.

J17. Field infiltration/seepage tests are critical to bridging our knowledge gap between transport processes at small scale and large-scale processes in complex fractured rock, and to gain of our confidence in site-scale modeling capabilities and results. A mesoscale infiltration and seepage test was conducted in a deep unsaturated fractured rock system by infiltration under ponded conditions in the upper-tunnel alcove and by collecting seepage at the lower-tunnel niche at Yucca Mountain. Spatial variabilities of infiltration and seepage rates were measured using multiple infiltration subplots and seepage trays. A three-dimensional unsaturated flow model was developed to reproduce the strong temporal and spatial variabilities in infiltration and seepage rates observed. Calibrated fracture permeability and van Genuchten α represent their respective spatial variabilities reflected in infiltration/seepage variabilities. The measured infiltration rates were found to be partially controlled by the fracture patterns on the infiltration plot, whereas no correlation was established between measured seepage rates and the density of fractures mapped on the niche ceiling. More importantly, numerous small fractures excluded in fracture mapping complicate such correlations, and the complexity of preferential unsaturated flow within the discrete fracture network can be attributed to the lack of correlation. The pervasive small fractures may be the key factor in the scale dependence of the effective matrix diffusion coefficient, as discussed above.

J19. Modeling and calibration of all processes relevant to on-site remediation are useful decision-support tools, particularly with respect to natural heterogeneity. A three-dimensional groundwater flow and advective transport model was developed at a heterogeneous, mountaineous site contaminated by DNAPL—in support of on-site remediation. The observed flow and plume conditions reflect the spatial variability in hydraulic conductivity and effective porosity. Calibration of these properties in several property zones was conducted. The calibrated effective porosity turns out to be much lower than the core porosity, indicating that only a small fraction of all pores are connected in the rock media. The calibrated flow properties combined with the measured boundary conditions can accurately reproduce the evolution of the dissolved DNAPL plume.

My additional research in this area includes the effects of heterogeneity on multiphase (DNAPL and water) flow, including the enhanced anisotropy of relative permeability by longer correlation length in the horizontal direction, and lateral spreading of DNAPL. This research will be extended to investigation of viscous fingering of phase CO_2 in hierarchical, multiscale, heterogeneous sedimentary sandstones for geologic carbon sequestration.